Electronic Supplementary Material (ESI) for Catalysis Science & Technology
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Supplementary Information for

Chromium(III) amine-bis(phenolate) complexes as catalysts for copolymerization of cyclohexene oxide and CO_2

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Table S1: Crystallographic and Structure Refinement Data for **$(1)_2$·LiCl·THF**.

Chemical formula	$C_{78}H_{110}Cl_3Cr_2LiN_2O_5 \cdot 2(C_7H_8)$
Colour	Green
Habit	Prism
Formula mass	1557.24
Crystal system	Trigonal
a, *b*, *c* [Å]	18.945(9), 18.945(9), 25.390(13)
α, *β*, *γ* [°]	90.00, 90.00, 120.00
Unit cell *V* [Å^3]	7892(7)
Temperature [K]	123(2)
Space group	$P3_1$ 2 1 (#152)
Z	3
D_c/g cm^{-3}	0.983
Radiation type	MoKα
Absorption, μ [cm^{-1}]	3.24
F(000)	2502
Reflections measured	73179
Independant refl's	7780
R_{int}	0.1281
R_1, $wR(F^2)$ (all)[a]	0.1351, 0.3327
R_1, $wR(F^2)$ $(I > 2\sigma(I))$ [b]	0.1211, 0.3154
Goodness of fit on F^2	1.187
CCDC Ref no.	974612

[a] $R_1 = \Sigma(|F_o| - |F_c|)/ \Sigma|F_o|)$. [b] $wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2)/ \Sigma w(F_o^2)^2]^{1/2}$.

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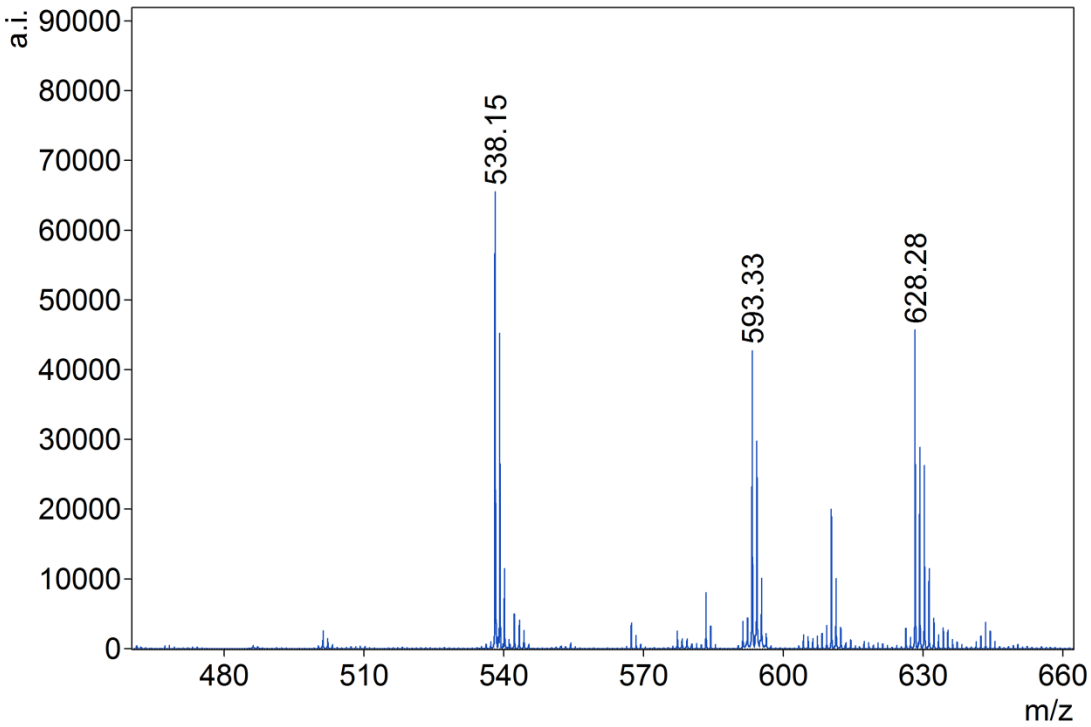

Figure S1. MALDI-TOF mass spectrum (lower mass region) of **1**.

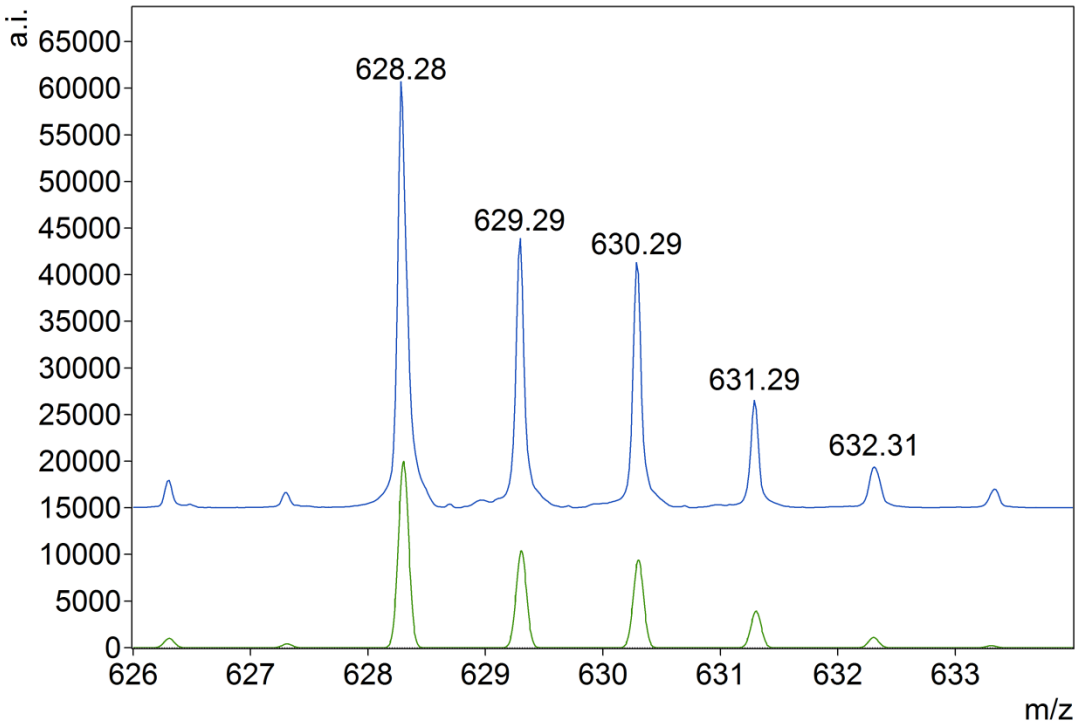

Figure S2. Experimental (upper) and theoretical (lower) MALDI-TOF isotopic distribution pattern for the $[M]^{+\cdot}$ peak of **1**.

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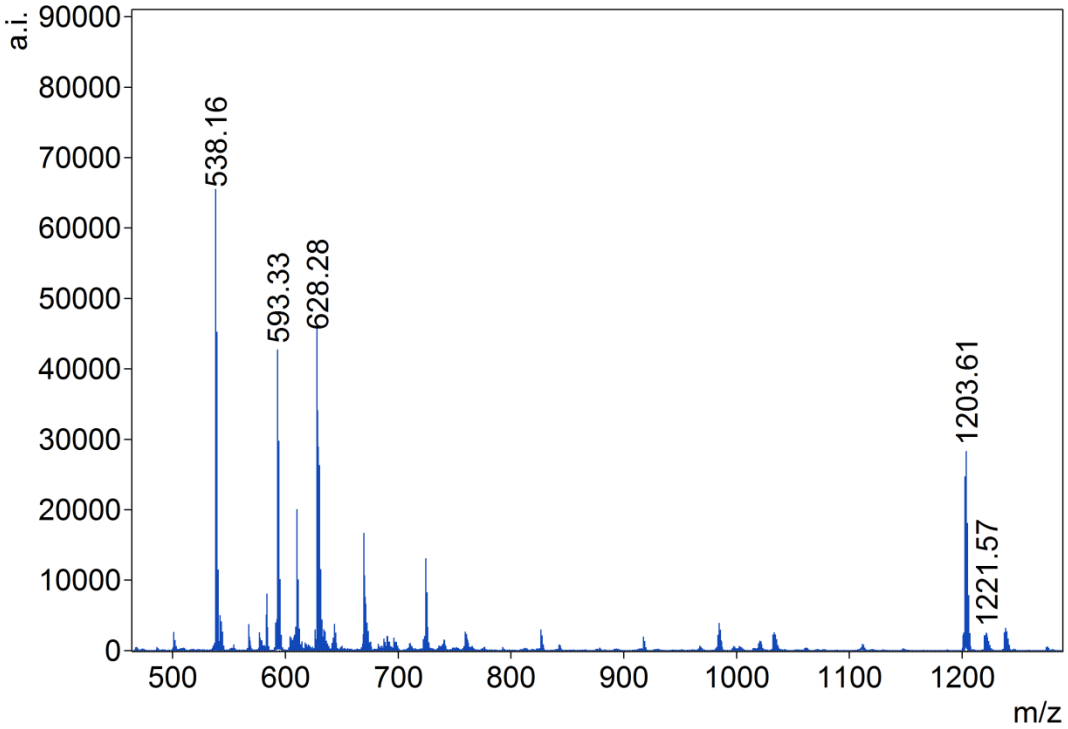

Figure S3. MALDI-TOF mass spectrum of **1** showing the higher mass region.

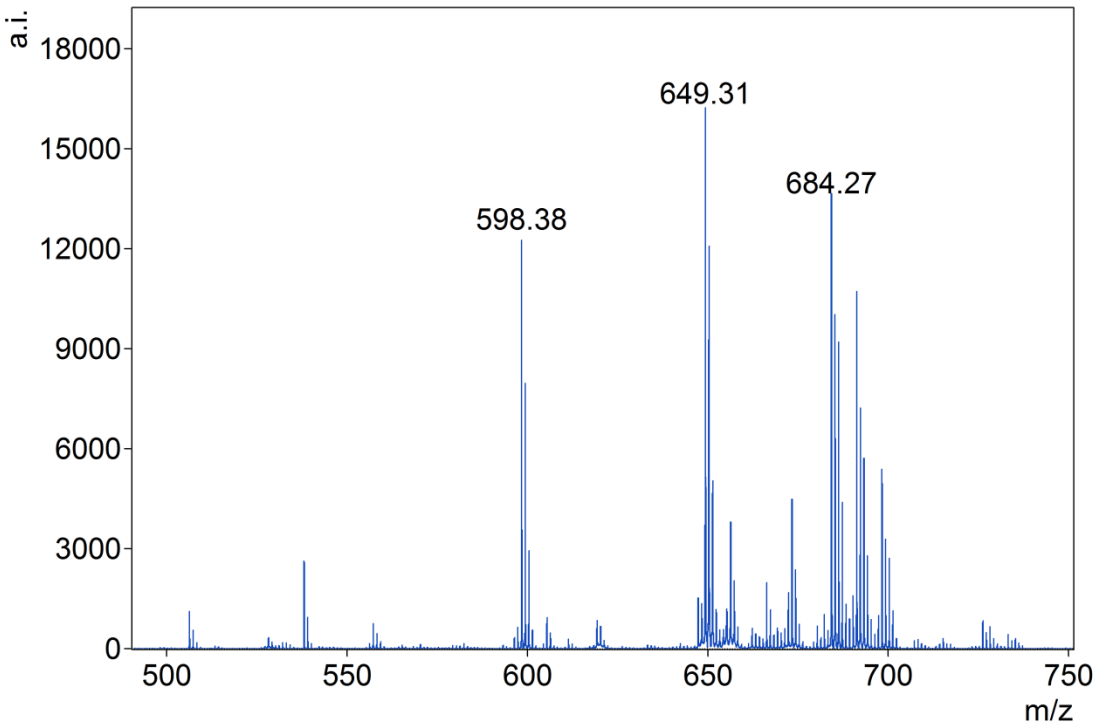

Figure S4. MALDI-TOF mass spectrum (lower mass region) of **2**.

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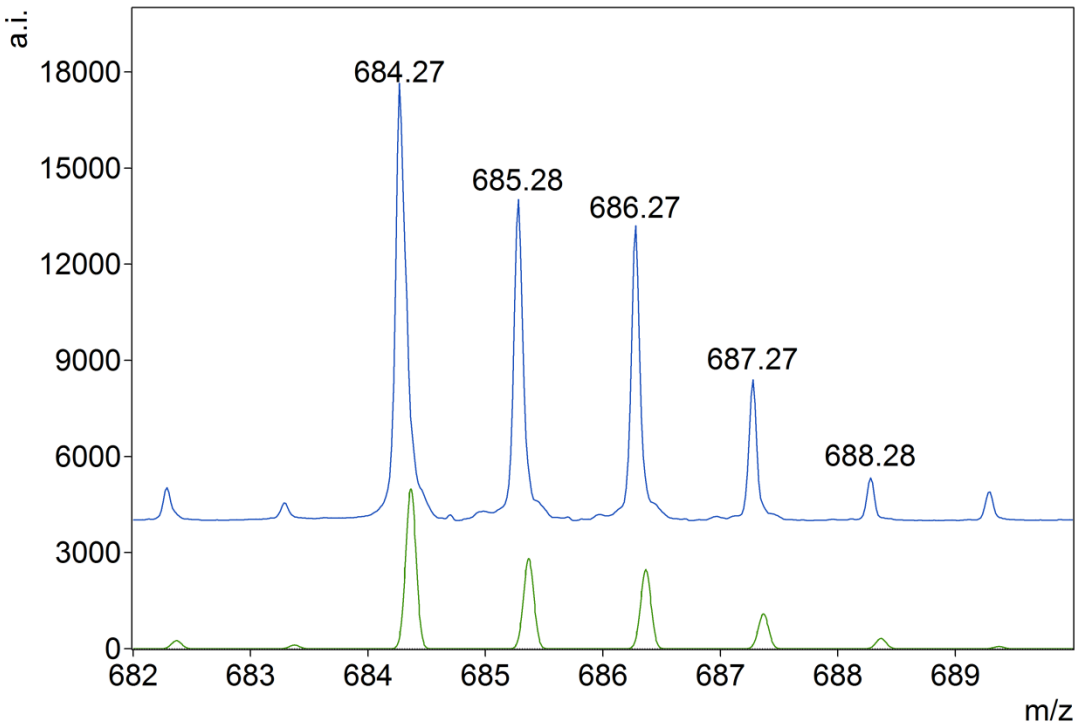

Figure S5. Experimental (upper) and theoretical (lower) MALDI-TOF isotopic distribution pattern for the molecular ion of the $[M]^{+\cdot}$ peak of **2**.

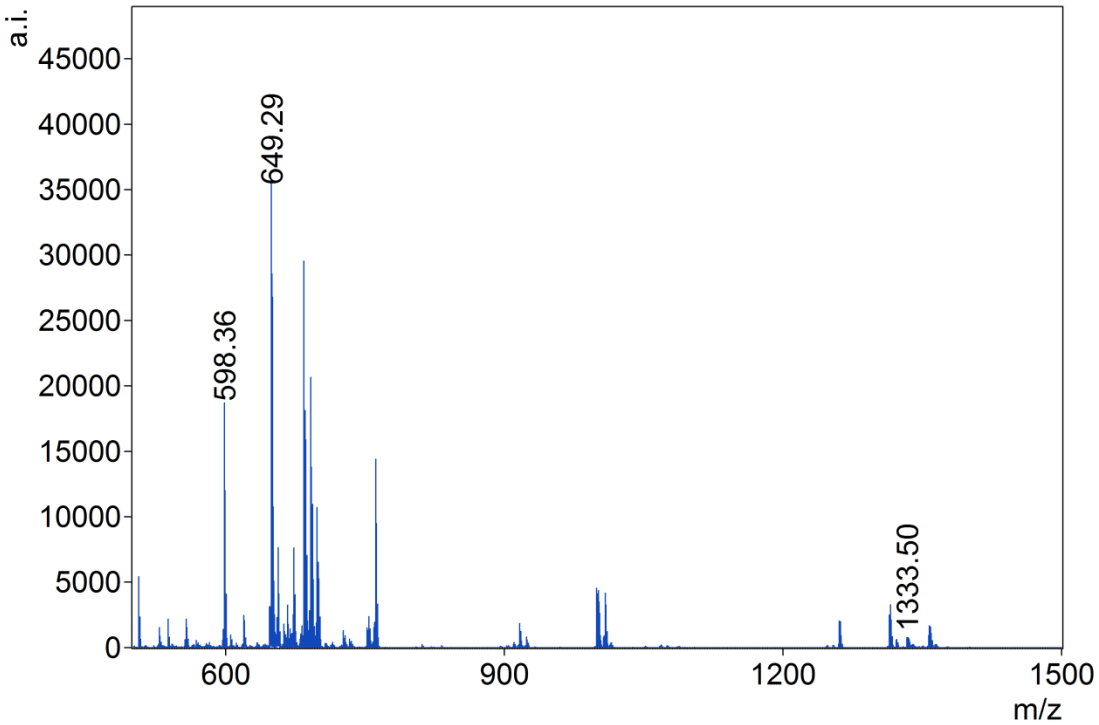

Figure S6. MALDI-TOF mass spectrum of **2** showing the higher mass region.

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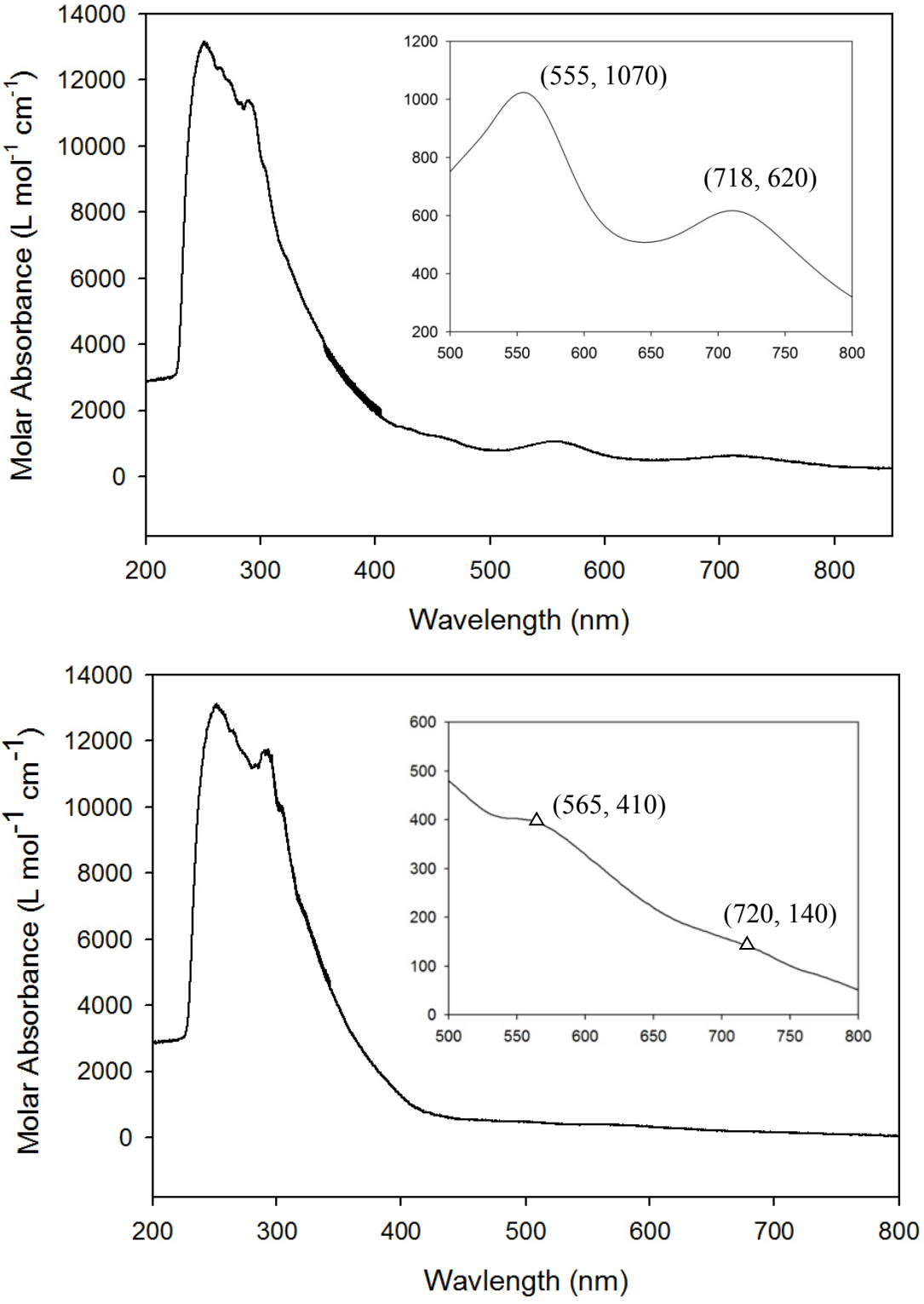

Figure S7. UV-Vis absorption spectrum of **1** (top) and **2** (bottom) in CH_2Cl_2. Insets: Expansions of visible regions showing peak wavelength and molar extinction coefficients.

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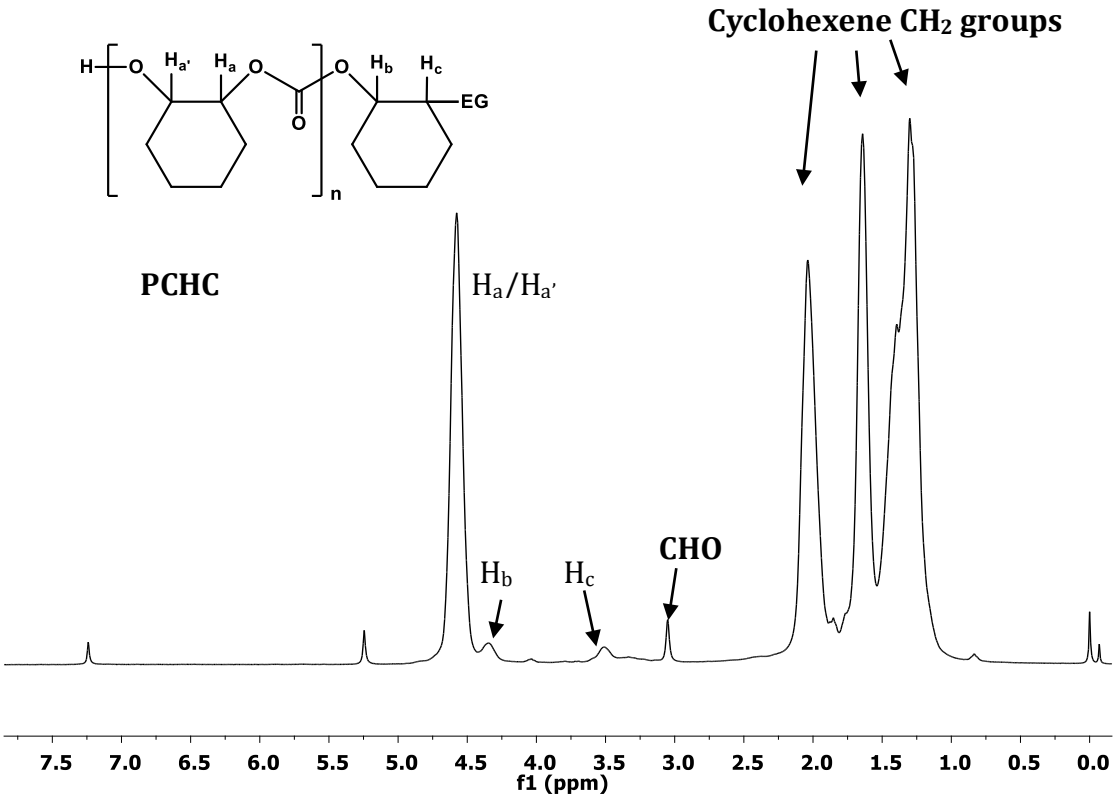

Figure S8. Typical ^{1}H NMR spectrum of PCHC in $CDCl_3$ (Table 2, entry 1), EG = end group.

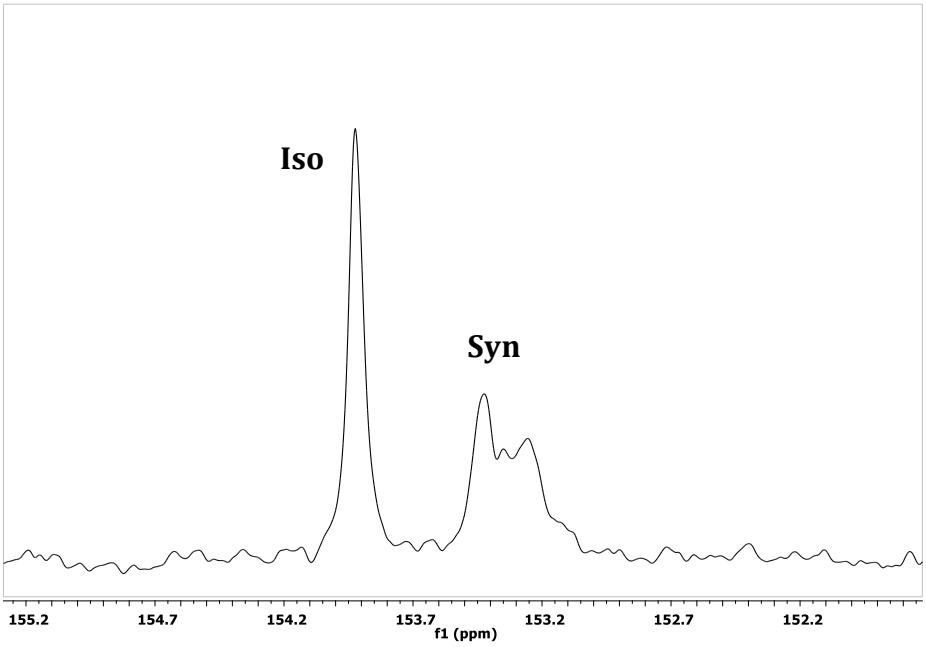

Figure S9. Carbonyl region of the ^{13}C NMR spectrum (75.5 MHz, $CDCl_3$) of PCHC prepared as described in Table 2, entry 1.

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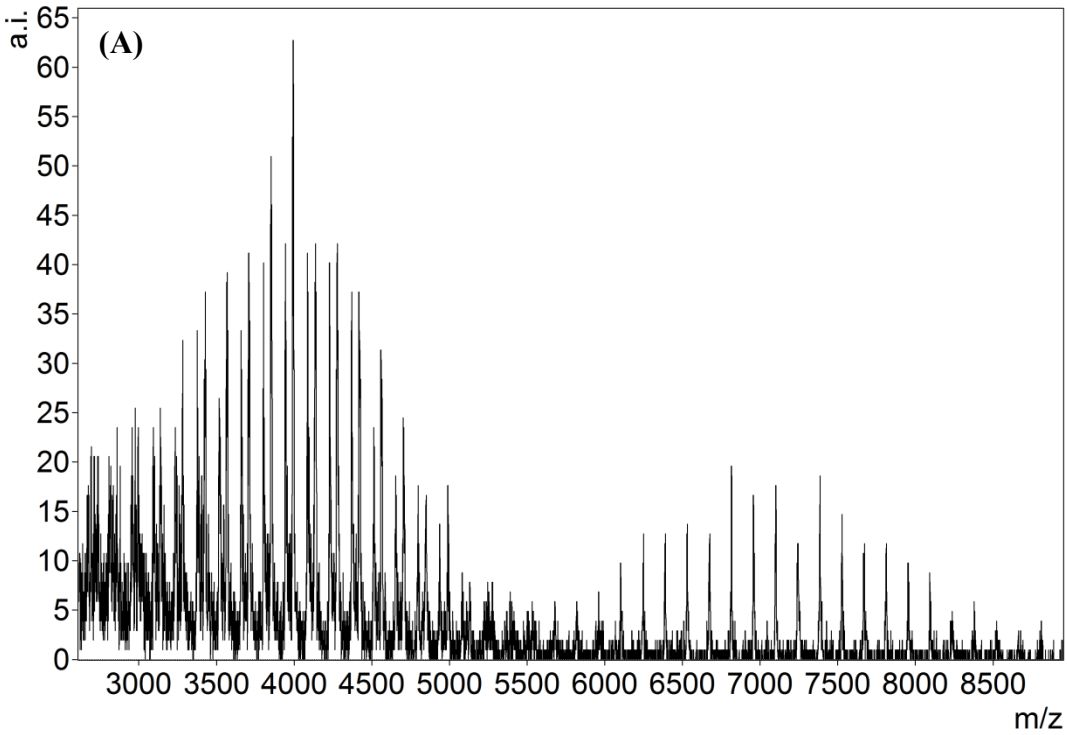

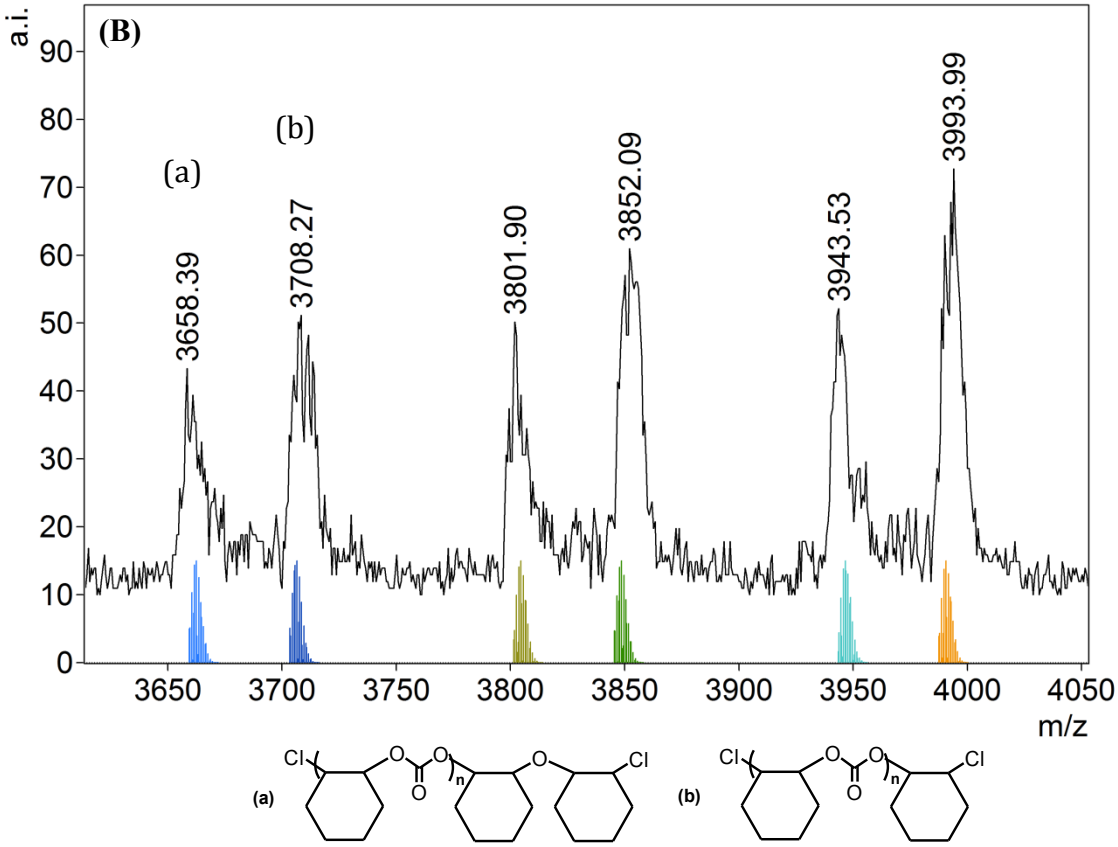

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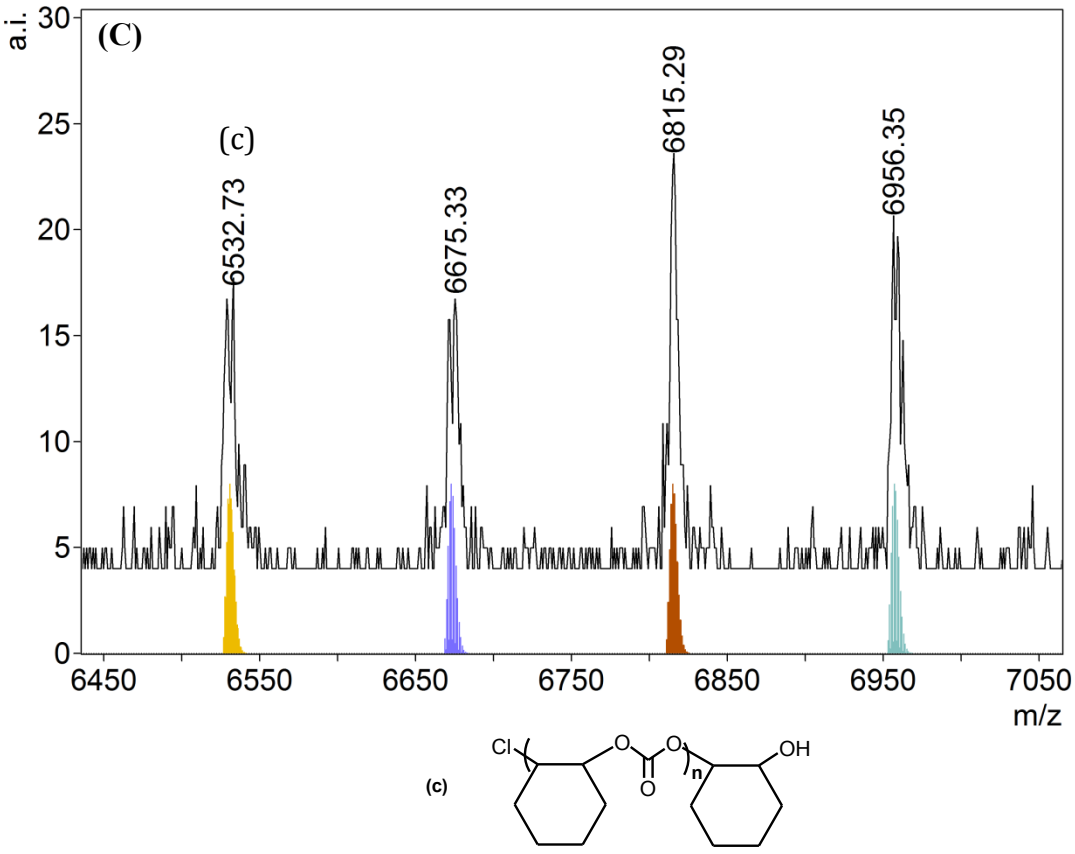

Figure S10. (A) MALDI-TOF MS of PCHC produced by **1** (Table 2, entry 4). (B) Magnified lower mass region of the spectrum (n = 24 – 27). (C) Magnified higher mass region of the spectrum (n = 45 – 48). Modeled isotopic masses and images for the polymer chains with end-groups (a), (b) and (c).

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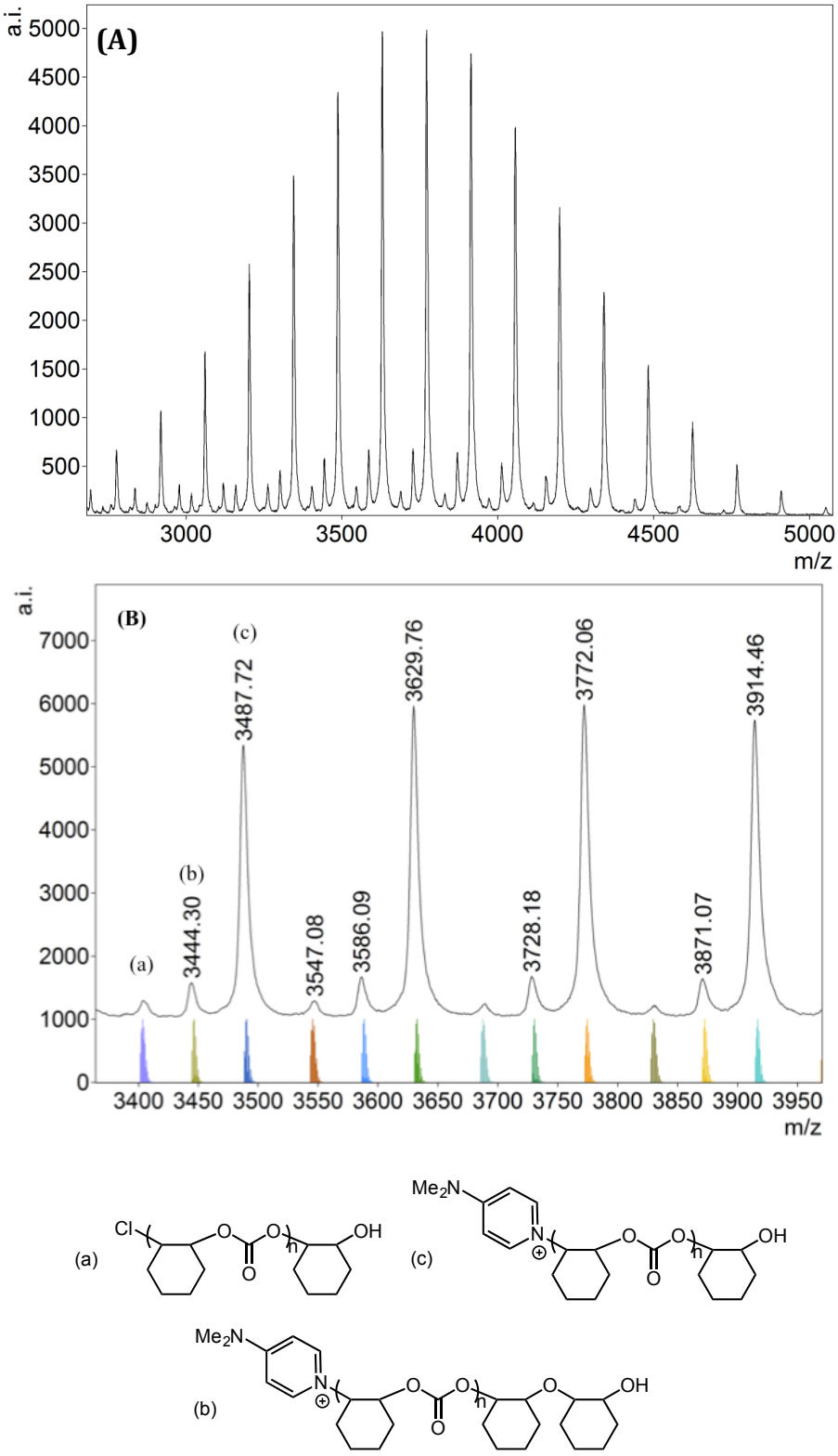

Figure S11. (A) MALDI-TOF MS of PCHC produced by **2** (Table 2, entry 5). (B) Magnified region of the spectrum (n = 22 – 25) and modeled isotopic masses and images for the polymer chains with end-groups (a) – (c).

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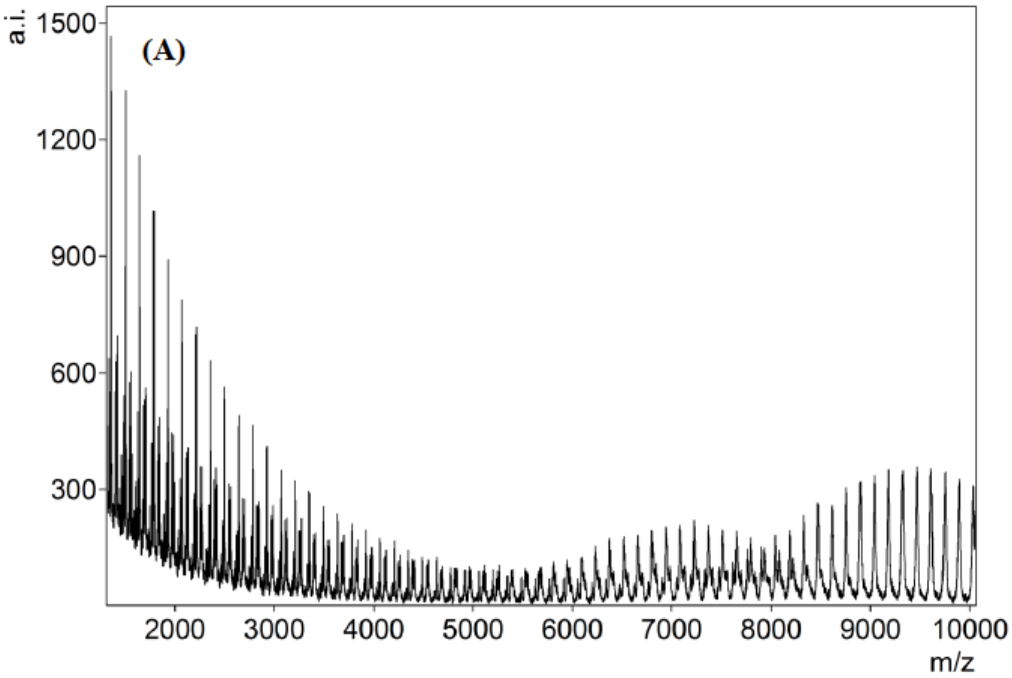

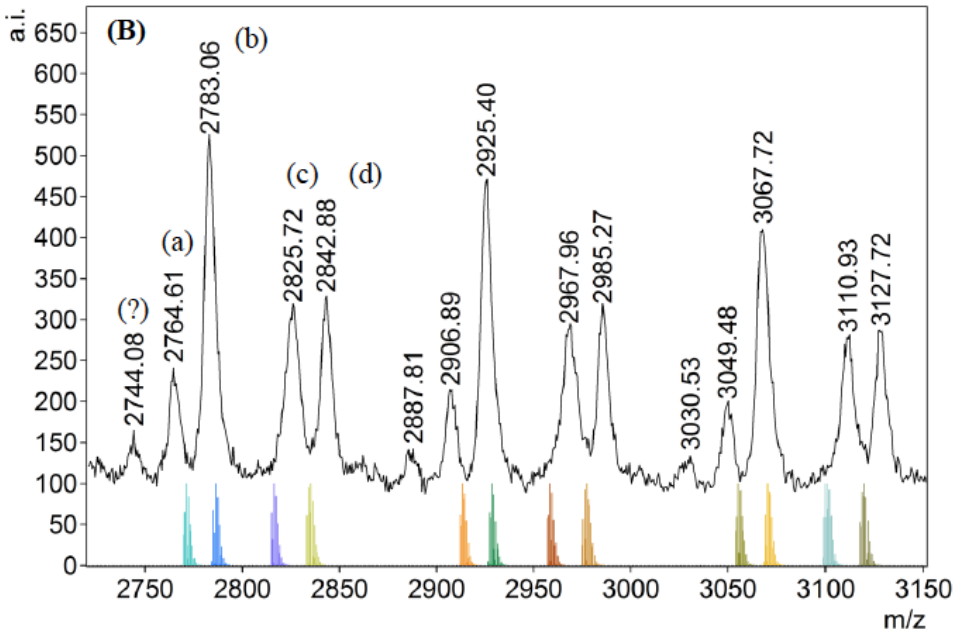

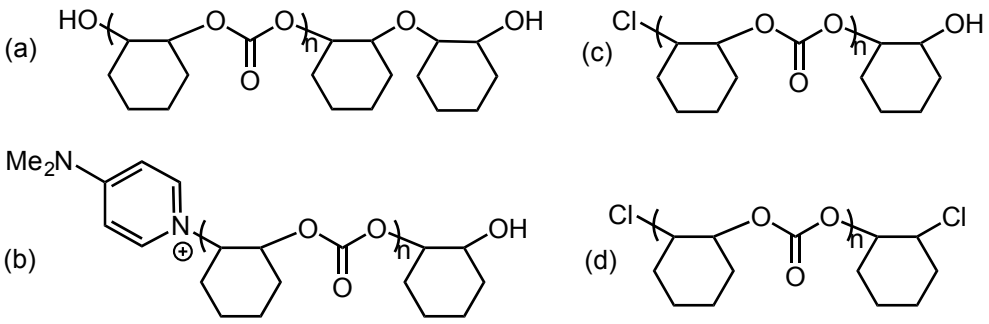

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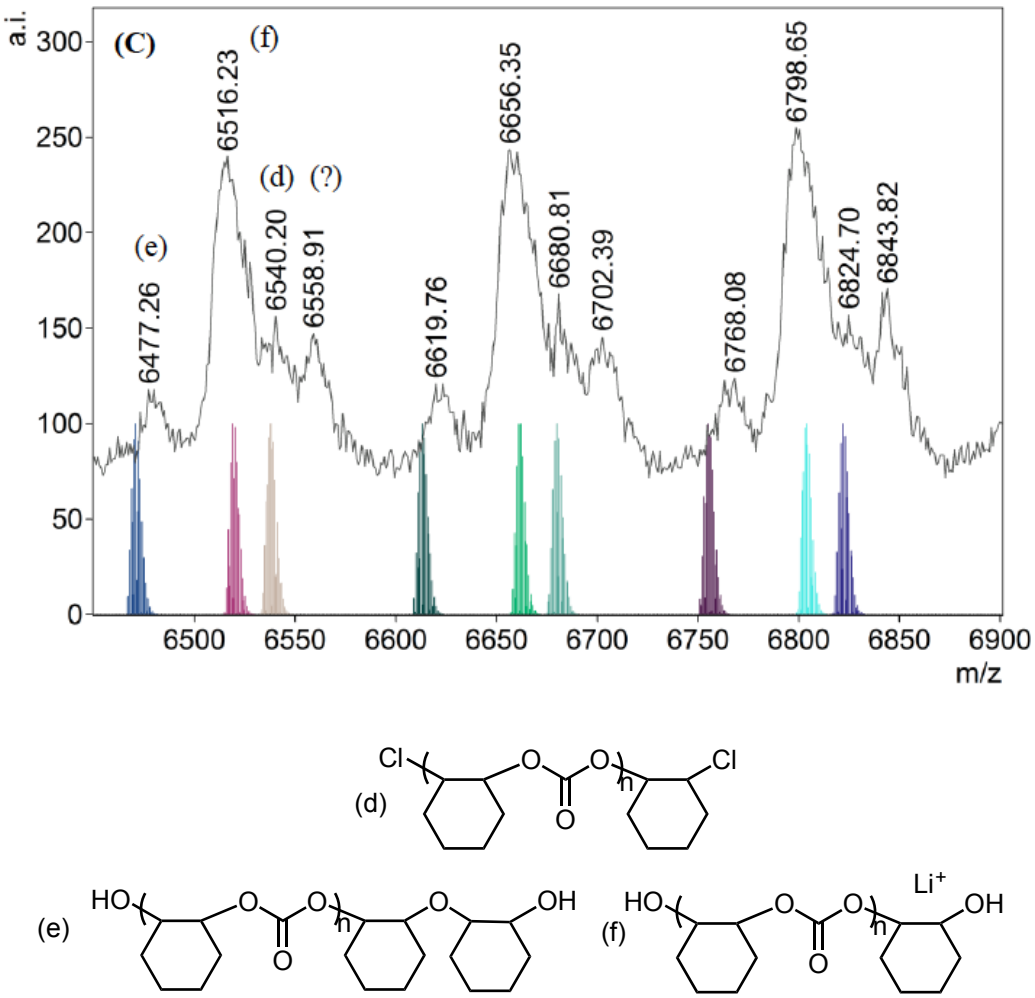

Figure S12. (A) MALDI-TOF MS of PCHC produced by **3** (Table 3, entry 1). (B) Magnified low molecular weight region of the spectrum (n = 18 – 20). (C) Magnified high molecular weight region of the spectrum (n = 44 – 47). Modeled isotopic masses and images for the polymer chains with end groups (a) – (f).

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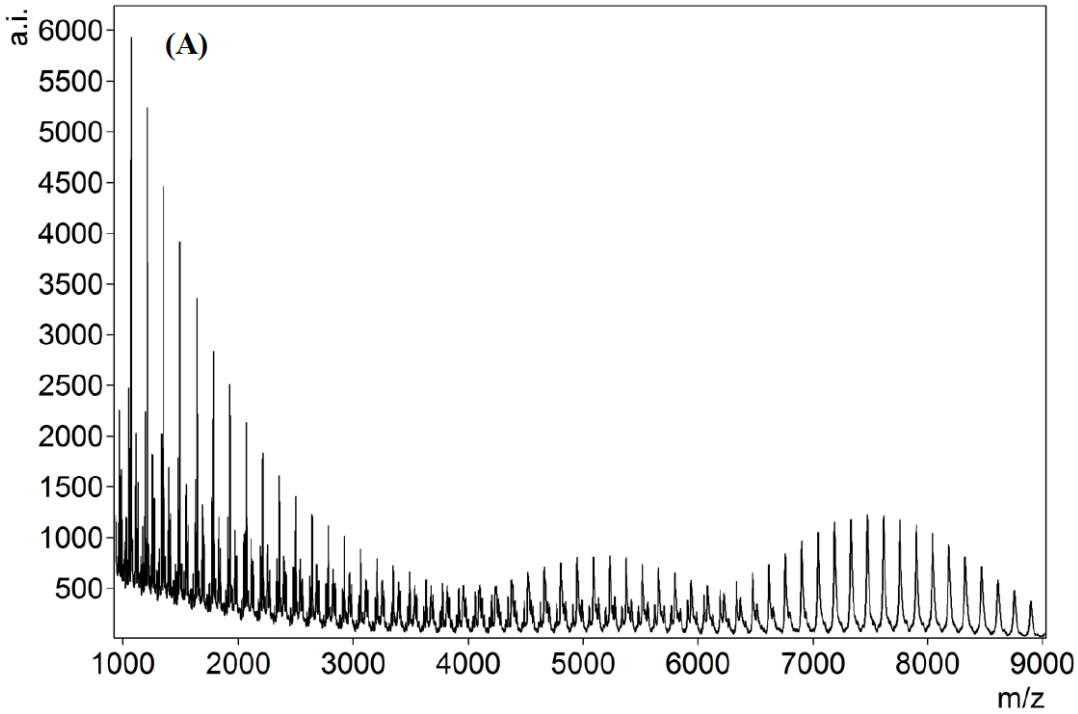

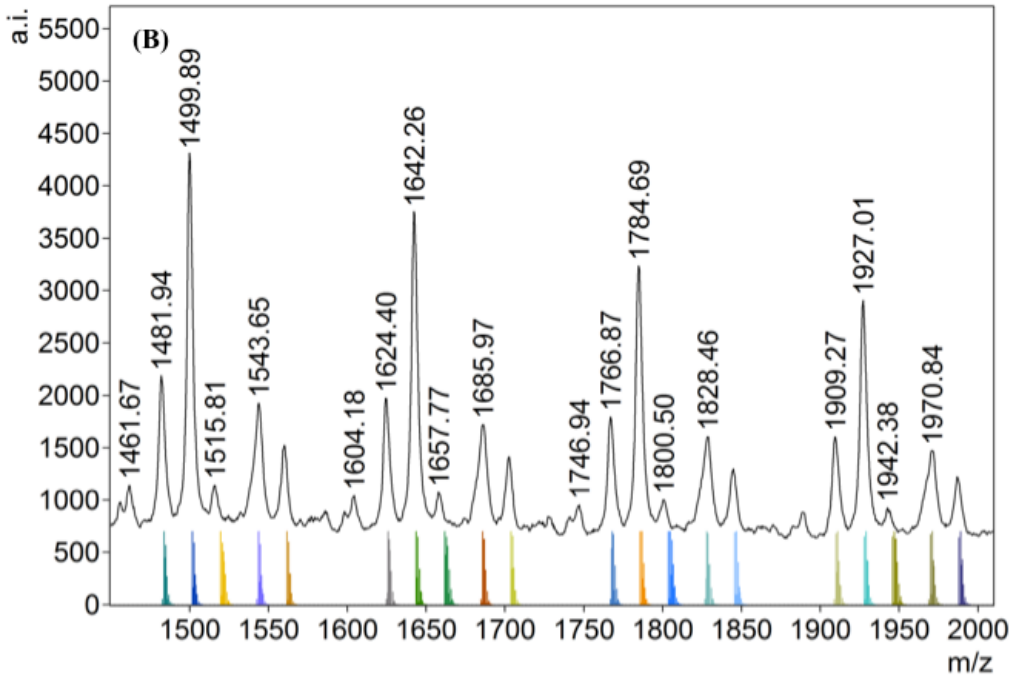

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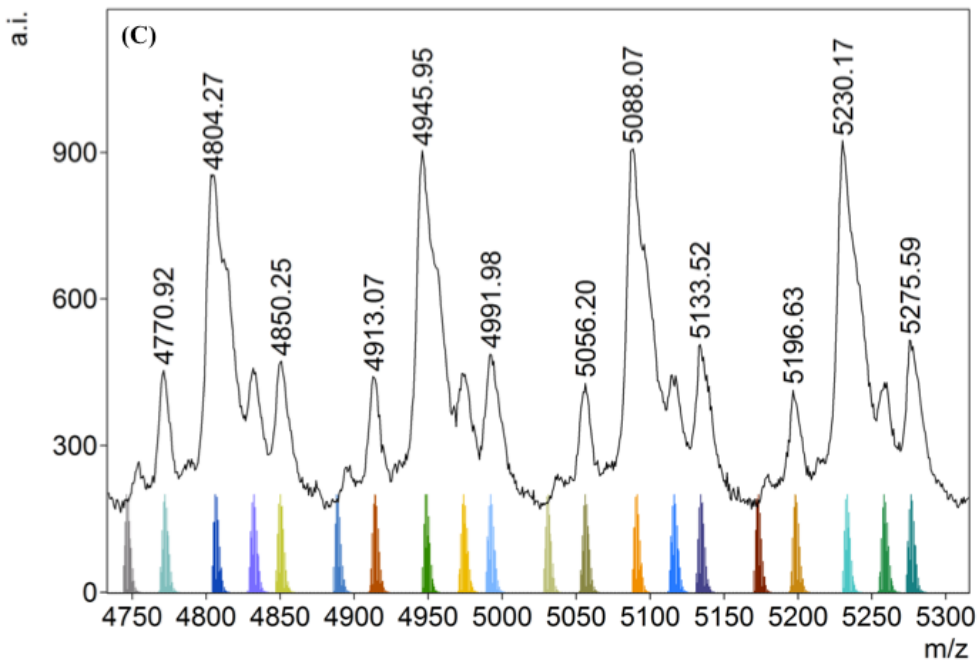

Figure S13. (A) MALDI-TOF MS of PCHC produced by **3** (Table 3, entry 5). (B) Magnified low molecular weight region of the spectrum (n = 9 – 11). (C) Magnified high molecular weight region of the spectrum (n = 32 – 35).